201-16554W

I U C L I D

Data Set

Existing Chemical	:	ID: 85507-79-5
CAS No.	:	85507-79-5
EINECS Name	:	Diundecyl phthalate
EC No.	:	287-401-6
TSCA Name	:	1,2-Benzenedicarboxylic acid, diundecyl ester, branched and linear
IUPAC Name	:	diundecyl phthalate, branched and linear
Molecular Weight	:	474
Molecular Formula	:	C3OH5OO4

Producer related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000

Substance related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000
Status	:	
Memo	:	ACC Phthalate Ester Panel HPV Testing Group
Printing date	:	07.12.2006
Revision date	:	
Date of last update	:	06.07.2006
Number of pages	:	24
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

Type	:	lead organisation
Name	:	ACC Phthalate Esters Panel HPV Testing Group
Contact person	:	Dr. Marian Stanley
Date	:	
Street	:	1300 Wilson Blvd.
Town	:	22209 Arlington, VA
Country	:	United States
Phone	:	(703) 741-5623
Telefax	:	(703) 741-6091
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

Remark : The American Chemistry Council Phthalate Esters Panel includes the following member companies:

BASF Corporation
CONDEA Vista Company
Eastman Chemical Company
ExxonMobil Chemical Company
Ferro Corporation
ICI Americas / Uniqema
Sunoco Chemicals
Teknor Apex Company

02.11.2001

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

Comment : This chemical is part of the High Molecular Weight Phthalate Esters subcategory. The subcategory includes eleven CAS numbers (see the Freetext Remark section for complete list).

Remark : This chemical is part of the High Molecular Weight Phthalate Esters subcategory. The subcategory includes the following eleven CAS numbers:
68648-93-1 1,2-benzenedicarboxylic acid, mixed decyl and hexyl and octyl diesters (610P)

117-84-0 1,2,-benzenedicarboxylic acid, dioctyl ester (DOP)

16883-83-3 1,2-Benzenedicarboxylic acid, benzyl 3-hydroxy-1-isopropyl-2,2-dimethylpropyl ester isobutyrate (B84P)

68515-40-2 1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl (B79P)

68515-45-7 1,2,-benzenedicarboxylic acid, dinonyl ester, branched and

linear (DNP)

68515-43-5 1,2-Benzenedicarboxylic acid, di-C9-11-branched and linear alkyl esters (911P)

84-77-5 1,2-benzenedicarboxylic acid, didecyl ester (DDP)

3648-20-2 1,2-benzenedicarboxylic acid, diundecyl ester (DUP)

85507-79-5 1,2-benzenedicarboxylic acid, di (C11) ester, branched and linear (DinUP)

111381-91-0 1,2-benzenedicarboxylic acid (C9, C11) ester, branched and linear (Din911P)

68515-47-9 1,2,-benzenedicarboxylic acid, di-C11-14-branched alkyl esters, C13 rich (DTDP)

The phthalate esters comprise a family of chemicals synthesized by esterifying phthalic anhydride with various alcohols in the presence of an acid catalyst. Phthalate esters are all 1,2-benzenedicarboxylic acids with side chain ester groups ranging from C1 to approximately C13. The structural characteristics of the ester side chains affect both the physical/chemical and biological properties of phthalate esters.

Phthalate esters are generally clear to yellow, oily liquids with high boiling ranges (>250oC) and low vapor pressures; properties which contribute to their high physical stability. They are readily soluble in most organic solvents and miscible with alcohol, ether and most oils. The aqueous solubility of phthalate esters is inversely related to their molecular weights. Lower molecular weight phthalates exhibit slight to moderate water solubility, whereas, higher molecular weight phthalates exhibit very low solubility.

The phthalate esters were subdivided into three subcategories based on their physicochemical and toxicological properties. The phthalate esters in this subcategory, High molecular weight phthalates, are produced from alcohols with straight-chain carbon backbones of >C7 or a ring structure.

Eleven of the U.S. HPV chemicals fall into this subcategory, which includes phthalates containing linear and branched diheptyl, dioctyl, dinonyl, didecyl, diundecyl, and ditridecyl alkyl groups. This subcategory also includes phthalates that can contain a benzyl group. Data for this subcategory were supplemented with published information on other phthalate esters currently being assessed under the OECD SIDS program, including di-isononyl (DINP) and di-isodecyl (DIDP) phthalate.

High molecular weight phthalates are used nearly exclusively as plasticizers of PVC. They are very insoluble in water, and have a very low vapor pressure. The extant database demonstrates that these substances have few biological effects.

08.05.2006

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type :

Substance type	:	organic
Physical status	:	liquid
Purity	:	
Colour	:	
Odour	:	

02.11.2001

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

Type of use	:	industrial
Category	:	Polymers industry
Remark	:	High molecular weight phthalates are used nearly exclusively as plasticizers of PVC.

02.11.2001

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value	:	= -9 °C
Decomposition	:	no, at °C
Sublimation	:	no
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	other TS: diundecyl phthalate ester (CAS No. 3648-20-2)
Remark	:	Data for diundecyl phthalate ester (CAS No. 3648-20-2) are used as read-across data to 1,2-benzenedicarboxylic acid, diundecyl ester, branched and linear (CAS No. 85507-79-5). Physicochemical data for 18 commercial phthalate esters from various sources including the public literature, manufacturing secifications, and handbook values were evaluated by an industry peer review process. Valid values were identified and presented in a phthalate ester environmental fate, peer reviewed publication. These data including the values for melting point represent the definitive and currently accepted physicochemical database for selected phthalate esters including diundecyl phthalate. There were no data on purity. Identified data sources included: Howard P, Banerjee S and Robillard K (1985). Measurement of water solubilities, octanol/water partition coefficients and vapor pressures of commercial phthalate esters. Environ. Tox. Chem 4, 653-661. Howear P (1989). Handbook of Environmental Fate and Exposure Data for Organic Chemicals: Vol I. Large Production and Priority Pollutants. Lewis Publishers, Inc., Chelsea, MI, USA. Sears J and Tourchette N (1982). Plasticizers, In: Kirk-Othmer Encyclopedia of Chemical Technology, Eds. Mark H, Othmer D, Overberger C and Seaborg G. Vol. 18, 3rd Edition. John Wiley and Sons, New York, NY, USA.
Test substance	:	diundecyl phthalate ester (CAS No. 3648-20-2)
Reliability	:	(2) valid with restrictions Although the original reference was not retrieved and reviewed for quality, this robust summary has a reliability rating of 2 because the data are from a peer reviewed database. The cited data are read-across from diundecyl phthalate ester (CAS No. 3648-20-2) to 1,2-benzenedicarboxylic acid, diundecyl ester, branched and linear (CAS No. 85507-79-5).
Flag	:	Critical study for SIDS endpoint
05.06.2006		(5)

Value	:	142 °C
Sublimation	:	no
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	other TS: 1,2-benzenedicarboxylic acid, diundecyl ester, branched and linear (CAS No. 85507-79-5)
Method	:	The calculated value was determined using MPBPWIN version 1.41, a subroutine within the computer program EPI SuiteTM version 3.12. Melting Point estimations performed by MPBPWIN are based on the average result of the calculation methods of K. Joback and Gold and Ogle. Joback's Method is described in Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds. The Gold and Ogle Method simply uses the formula Tm = 0.5839Tb, where Tm is the melting point in Kelvin and Tb is the

boiling point in Kelvin.
The SMILES notation used in the calculation was:
O=C(c1ccccc1C(=O)OCCCCCCCCCCC)OCC(C(CC)CCC)CCC

Remark : EPI SuiteTM is used by the US EPA for estimating chemicophysical properties of substances. However, the melting point calculation in EPI SuiteTM provides erroneously high results for phthalate esters.

Test substance : 1,2-benzenedicarboxylic acid, diundecyl ester, branched and linear (CAS No. 85507-79-5)

Reliability : (3) invalid

05.06.2006 (2)

2.2 BOILING POINT

Value : 498 °C at 1013 hPa
Decomposition : no
Method : other: calculated
Year :
GLP :
Test substance : other TS: 1,2-benzenedicarboxylic acid, diundecyl ester, branched and linear (CAS No. 85507-79-5)

Method : Boiling point calculated by MPBPWIN subroutine in EPI SuiteTM, which is based on the method of S. Stein and R. Brown in "Estimation of Normal Boiling Points from Group Contributions". 1994. J. Chem. Inf. Comput. Sci. 34: 581-587.
The SMILES notation used in the calculation was:
O=C(c1ccccc1C(=O)OCCCCCCCCCCC)OCC(C(CC)CCC)CCC

Remark : EPI SuiteTM is used by the US EPA for estimating chemicophysical properties of substances.

Test substance : 1,2-benzenedicarboxylic acid, diundecyl ester, branched and linear (CAS No. 85507-79-5)

Reliability : (2) valid with restrictions
The value was calculated based on chemical structure as modeled by EPI SuiteTM. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

Flag : Critical study for SIDS endpoint

05.06.2006 (2)

2.3 DENSITY

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : = .00000000497 hPa at 25 °C
Decomposition : no
Method : other (calculated)
Year :
GLP :
Test substance : other TS: 1,2-benzenedicarboxylic acid, diundecyl ester, branched and linear (CAS No. 85507-79-5)

Remark : Physicochemical data for 22 selected commercial phthalate esters from various sources including the public literature, manufacturing secifications, handbook values, and computer modeling were evaluated by an industry

peer review process. Valid values were identified and presented in a phthalate ester physicochemical properties, peer reviewed publication. These data including the values for vapour pressure represent the definitive and currently accepted physicochemical database for selected phthalate esters including diundecyl phthalate.

Quantitative structure-property relationships, significant at the 99.9% level, were developed using the relevant phthalate ester data to estimate solubility in water, air, and octanol, where V = the Le Bas molar volume (cm3 mol-1). The Le Bas molar volume used for diundecyl phthalate ester was 653.6 cm3 mol-1.

Log CS(WL) = -0.012V + 5.8, n = 35 (solubility in water)
r2 = 0.98, SE = 0.39

Log CS(AL) = -0.013V - 1.3, n = 15 (solubility in air)
r2 = 0.87, SE = 0.33

Log CS(OL) = -0.016V + 3.4, n = 68 (solubility in octanol)
r2 = 0.19, SE = 0.41

It was recommended by the authors that the above regressions be used for predicting the three solubilities for phthalate esters with alkyl chain lengths from 1 to 13 carbons.

Test substance : 1,2-benzenedicarboxylic acid, diundecyl ester, branched and linear (CAS No. 85507-79-5)

Reliability : (2) valid with restrictions
The value was calculated based on the QSPR (quantitative structure-property relationship) three-solubility model. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

Flag : Critical study for SIDS endpoint
05.06.2006 (1)

Value : = .00000000271 hPa at 25 °C
Decomposition : no
Method : other (calculated)
Year :
GLP :
Test substance : other TS: 1,2-benzenedicarboxylic acid, diundecyl ester, branched and linear (CAS No. 85507-79-5)

Method : Calculated values using MPBPWIN version 1.41, a subroutine of the computer program EPI SuiteTM version 3.12.
Vapor Pressure estimations performed by MPBPWIN are based on the calculation method of Grain, which uses boiling point (498°C at 1013 hPa) for the calculation.
A modified Grain Method is described on page 31 of Neely and Blau's Environmental Exposure from Chemicals, Volume 1, CRC Press. 1985.
The SMILES notation used in the calculation was:O=C(c1ccccc1C(=O)OCCCCCCCCCCC)OCC(C(CC)CCC)CCC

Remark : EPI SuiteTM is used by the US EPA for estimating chemicophysical properties of substances.

Test substance : 1,2-benzenedicarboxylic acid, diundecyl ester, branched and linear (CAS No. 85507-79-5)

Reliability : (2) valid with restrictions
05.06.2006 (2)

2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water

Log pow	:	= 10.33 at 25 °C
pH value	:	
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	other TS: 1,2-benzenedicarboxylic acid, diundecyl ester, branched and linear (CAS No. 85507-79-5)
Remark	:	Physicochemical data for 22 selected commercial phthalate esters from various sources including the public literature, manufacturing secifications, handbook values, and computer modeling were evaluated by an industry peer review process. Valid values were identified and presented in a phthalate ester physicochemical properties, peer reviewed publication. These data including the values for octanol-water partitioning represent the definitive and currently accepted physicochemical database for selected phthalate esters including diundecyl phthalate. Quantitative structure-property relationships, significant at the 99.9% level, were developed using the relevant phthalate ester data to estimate solubility in water, air, and octanol, where V = the Le Bas molar volume (cm3 mol-1). The Le Bas molar volume used for diundecyl phthalate ester was 653.6 cm3 mol-1. Log CS(WL) = -0.012V + 5.8, n = 35 (solubility in water) r2 = 0.98, SE = 0.39 Log CS(AL) = -0.013V - 1.3, n = 15 (solubility in air) r2 = 0.87, SE = 0.33 Log CS(OL) = -0.016V + 3.4, n = 68 (solubility in octanol) r2 = 0.19, SE = 0.41 It was recommended by the authors that the above regressions be used for predicting the three solubilities for phthalate esters with alkyl chain lengths from 1 to 13 carbons.
Test substance	:	1,2-benzenedicarboxylic acid, diundecyl ester, branched and linear (CAS No. 85507-79-5)
Reliability	:	(2) valid with restrictions The value was calculated based on the QSPR (quantitative structure-property relationship) three-solubility model. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint
05.06.2006		(1)
Partition coefficient	:	octanol-water
Log pow	:	11.83 at 25 °C
pH value	:	
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	other TS: 1,2-benzenedicarboxylic acid, diundecyl ester, branched and linear (CAS No. 85507-79-5)
Method	:	The value was calculated using KOWWIN version 1.67, a subroutine of the computer program EPI SuiteTM version 3.12. Octanol / Water Partition Coefficient estimations performed by KOWWIN are based on an atom/fragment contribution method of W. Meylan and P. Howard in "Atom/fragment contribution method for estimating octanol-water partition coefficients". 1995. J. Pharm. Sci. 84:83-92. The SMILES notation used in the calculation was: O=C(c1ccccc1C(=O)OCCCCCCCCCCC)OCC(C(CC)CCC)CCC
Remark	:	EPI SuiteTM is used and advocated by the US EPA for chemical property

estimation.

Test substance : 1,2-benzenedicarboxylic acid, diundecyl ester, branched and linear (CAS No. 85507-79-5)

Reliability : (2) valid with restrictions
The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

05.06.2006 (2)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	= .00441 other: ug/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	other TS: 1,2-benzenedicarboxylic acid, diundecyl ester, branched and linear (CAS No. 85507-79-5)

Remark : Physicochemical data for 22 selected commercial phthalate esters from various sources including the public literature, manufacturing secifications, handbook values, and computer modeling were evaluated by an industry peer review process. Valid values were identified and presented in a phthalate ester physicochemical properties, peer reviewed publication. These data including the values for water solubility represent the definitive and currently accepted physicochemical database for selected phthalate esters including diundecyl phthalate.

Quantitative structure-property relationships, significant at the 99.9% level, were developed using the relevant phthalate ester data to estimate solubility in water, air, and octanol, where V = the Le Bas molar volume (cm3 mol-1). The Le Bas molar volume used for diundecyl phthalate ester was 653.6 cm3 mol-1.

Log CS(WL) = -0.012V + 5.8, n = 35 (solubility in water)
r2 = 0.98, SE = 0.39

Log CS(AL) = -0.013V - 1.3, n = 15 (solubility in air)
r2 = 0.87, SE = 0.33

Log CS(OL) = -0.016V + 3.4, n = 68 (solubility in octanol)
r2 = 0.19, SE = 0.41

It was recommended by the authors that the above regressions be used for predicting the three solubilities for phthalate esters with alkyl chain lengths from 1 to 13 carbons.

Test substance : 1,2-benzenedicarboxylic acid, diundecyl ester, branched and linear (CAS No. 85507-79-5)

Reliability : (2) valid with restrictions
The value was calculated based on the QSPR (quantitative structure-property relationship) three-solubility model. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

Flag	:	Critical study for SIDS endpoint
05.06.2006		(1)
Solubility in	:	Water
Value	:	= .00007 other: ug/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other
Year	:	
GLP	:	
Test substance	:	other TS: 1,2-benzenedicarboxylic acid, diundecyl ester, branched and linear (CAS No. 85507-79-5)
Method	:	Water solubility calculated by WSKOWWIN, a subroutine of the computer program EPI SuiteTM version 3.12. that is based on a Kow correlation method described by W. Meylan, P. Howard and R. Boethling in "Improved method for estimating water solubility from octanol/water partition coefficient". Environ. Toxicol. Chem. 15:100-106. 1995. The SMILES notation used in the calculation was: O=C(c1ccccc1C(=O)OCCCCCCCCCCC)OCCCCCCCCCCC
Remark	:	EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.
Test substance	:	1,2-benzenedicarboxylic acid, diundecyl ester, branched and linear (CAS No. 85507-79-5)
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
05.06.2006		(2)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	Sun light
Light spectrum	:	nm
Relative intensity	:	1 based on intensity of sunlight
Conc. of substance	:	at 25 °C
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000 molecule/cm³
Rate constant	:	= .00000000003185 cm³/(molecule*sec)
Degradation	:	= 50 % after 4 hour(s)
Deg. product	:	not measured
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	other TS: 1,2-benzenedicarboxylic acid, diundecyl ester, branched and linear (CAS No. 85507-79-5)
Method	:	Calculated values using AOPWIN version 1.91, a subroutine of the computer program EPI SuiteTM version 3.12. Indirect photodegradation, or atmospheric oxidation potential, is based on the structure-activity relationship methods developed by R. Atkinson.
Remark	:	50% degradation after 4.0 hrs or 0.33 days based on a 12-hour day. The computer program AOPWIN (atmospheric oxidation program for Microsoft Windows) (EPI SuiteTM, 2000) calculates a chemical half-life for a 12-hour day (the 12-hour day half-life value normalizes degradation to a standard day light period during which hydroxyl radicals needed for degradation are generated), based on an OH- reaction rate constant and a defined OH- concentration. EPI SuiteTM is used by the US EPA for estimating chemicophysical properties of substances.
Test substance	:	1,2-benzenedicarboxylic acid, diundecyl ester, branched and linear (CAS No. 85507-79-5)
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPI SuiteTM. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

06.07.2006 (2)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	at °C
t1/2 pH7	:	6.3 year at 25 °C
t1/2 pH9	:	- at °C
Deg. product	:	not measured
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	other TS: 1,2-benzenedicarboxylic acid, diundecyl ester, branched and linear (CAS No. 85507-79-5)
Method	:	Hydrolysis rate calculated by HYDROWIN ver. 1.67, a subroutine of the computer program EPI SuiteTM version 3.12, that is based on work for EPA by T. Mill et al.

Remark	:	EPI SuiteTM is used by the US EPA for estimating chemicophysical properties of substances.
Test substance	:	1,2-benzenedicarboxylic acid, diundecyl ester, branched and linear (CAS No. 85507-79-5)
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPI SuiteTM. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

05.06.2006 (2)

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3.3.2 DISTRIBUTION

Media	:	air - biota - sediment(s) - soil - water
Method	:	Calculation according Mackay, Level I
Year	:	1997
Method	:	The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment. Physicochemical input values for the model to represent a diundecyl phthalate ester were: MW = 474.7 Temperature = 25C Water Solubility = 0.0000044 mg/L Vapor Pressure = 4.97E-7 Pa Pow = 10.3 Melting Point = -9C Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, sediment, suspended sediment, biota).
Result	:	Soil = 97.7% Air = 0.0% Water = 0.0% Sediment = 2.2% Suspended sed. = 0.1% Biota = 0.0%
Test substance	:	1,2-benzenedicarboxylic acid, diundecyl ester, branched and linear (CAS No. 85507-79-5)
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated and not measured.

Flag : Critical study for SIDS endpoint
05.06.2006 (4)

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level III
Year :

Remark : Physicochemical input values for the model to represent a diundecyl phthalate ester were:
MW = 474.7
Temperature = 25C
Water Solubility = 0.0000044 mg/L
Vapor Pressure = 4.97E-7 Pa
Pow = 10.3
Melting Point = -9C

Emissions rates used in the calculation (default valutes):

Compartment	Rate (kg/hr)
Air	1000
Water	1000
Soil	1000

Half-lives used in the calculation:

Compartment	Half-life (hr)
Air	4.0a
Water	240b
Soil	840c
Sediment	840c

a - as calculated using AOPWIN version 1.91, a subroutine of the computer program EPI SuiteTM version 3.12 [Environmental Protection Agency (EPA) (2000). EPI SuiteTM, Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.]

b - based on biodegradation data from EBSI (1995) and Boethling (2000): Exxon Biomedical Sciences, Inc. (1995). Ready Biodegradability, Manometric Respirometry. Study No. 199894A. Unpublished report.

Boethling R (2000). HPVC-Screening Tool: Using Ready and Inherent Biodegradability Data to Derive Input Data for the EQC Model, Appendix 10 in Environment Canada, Environmental Categorization for Persistence Bioaccumulation and Inherent Toxicity of Substances on the Domestic Substance List Using QSARs, Results of an international workshop hosted by Chemicals Evaluation Division of Environment Canada, Nov. 11-12, 1999, in Philadelphia, PA, USA.

c - based on Boethling, R. recommendation that half-lives of 3 to 4 times longer than surface water should be used for soil and sediment.

Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, sediment).

Result : Using the Mackay Level I calculation, the following distribution is predicted for diundecyl phthalate ester:

Compartment	%Distribution
Air	0.4
Water	5.4

		Soil 65.3 Sediment 28.9
Test substance	:	1,2-benzenedicarboxylic acid, diundecyl ester, branched and linear (CAS No. 85507-79-5)
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated.

05.06.2006 (3)

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

(1) Cousins I and Mackay D (2000). Correlating the physical-chemical properties of phthalate esters using the 'three solubility' approach. Chemosphere 41, 1389-1399.

(2) Environmental Protection Agency (EPA) (2000). EPI SuiteTM, Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.

(3) Mackay D (1998). Level III Fugacity-Based Environmental Equilibrium Partitioning Model, Version 2.1 (16-bit). Environmental Modelling Centre, Trent University, Ontario, Canada.

(4) Mackay D, DiGuardo A, Paterson S and Cowan C (1997). EQC Model ver. 1.01, available from the Environmental Centre, Trent University, Canada.

(5) Staples C, Peterson D, Parkerton T and Adams W (1997). The environmental fate of phthalate esters: A literature review. Chemosphere 35, 667-749.

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

Memo : This chemical is part of the High Molecular Weight Phthalate Esters subcategory. Data from other chemicals in this subcategory can be used to assess the potential hazards of all category members.

Remark : Chapters 2, 3, 4 & 5

There are measured physicochemical property data available for some of the higher phthalates. Computer estimation models were also used to calculate physicochemical and fate data for phthalates in this subcategory. The calculated data were developed from a computer model used by the EPA, as cited in an EPA guidance document prepared for the HPV Challenge Program. Depending upon the endpoint, the modeled data agree with measured data. The combination of measured values and calculated values is sufficient to provide the required information on the physiochemical and fate properties of the HPV phthalates in the high molecular weight subcategory.

A complete health effects SIDS data set is available for diisononyl (DINP) and diisodecyl (DIDP) phthalates. These substances are under review in Europe as part of the Existing Substances Risk Assessment, and have been included as reference compounds for the high molecular weight phthalate subcategory. Although not complete, health effects data are also available for many of the HPV substances in this subcategory. These phthalates all demonstrate minimal acute toxicity, are not genotoxic, exhibit some liver and kidney effects at high doses, and are negative for reproductive and developmental effects. Further, the available data indicate that the toxicological activity of these molecules diminishes with increasing molecular weight. The available data, supplemented with the data from the reference compounds (DINP, DIDP), are believed to be sufficient to use as read-across to the other category members, with side chains in the C7 - C13 range.

Ecotoxicity test data in fish, daphnia, and algae are available for 610P, 711P, DINP, DUP, DIDP and DTDP. These phthalates all contain alkyl chain lengths in the range of C7 to C13. The remaining members of this subgroup are all various mixtures of C7 through C11 alkyl chain isomers. All of the measured data for these higher phthalates show no effects on acute or chronic exposure to aquatic organisms. As with DIOP and DEHP, the higher phthalates are too insoluble to have acute or chronic toxicity.

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10.3 RISK ASSESSMENT